Modeling the impact of strain on color centers in diamond: a first principles study of the GeV-center

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Color centers in diamond have always carried the human interest, though the reason has changed over time. Today, this interest is founded in high-tech applications such as quantum information technology and nano-sensing.[1] Although a plethora of color centers has experimentally been detected, only few have been fully and decisively structurally characterised.[2-5] With regard to the high-tech applications mentioned above, the NV-center is probably the most widely studied and best characterized color center in theoretical diamond research, since its creation in experiments is very well controlled these days. Despite its popularity, it is also know not to be the most suitable candidate for these applications due to the presence of a very strong phonon sideband which reduces the relative intensity of the zero-phonon-line (ZPL). Group-IV color centers in contrast are know to show a better Debye-Waller factor, making them much more suitable for future applications. In this work, we present a quantum mechanical study of the GeV-color center in diamond. We investigate the impact of strain and defect concentration on the ZPL as these will help to elucidate the experimental observation of these ZPL in nanocrystalline diamond films.

GeV-color centers in diamond

Although the basic structure of the GeV-color center is known as a "split-vacancy" defect, the impact of strain and concentration is not as well established. We have modelled the GeV-color center for concentrations ranging from 0.1% (1000 atom conventional supercell) to 1.5% (64 atom conventional supercell) using first principles calculations (*c.q.* Density Functional Theory using hybrid functionals for high accuracy electronic structure results). At each concentration, the supercells cells were strained both isotropic and anisotropic to mimic the possible experimental conditions experienced in nanocrystalline films. The impact of the strain on the local charge distribution was investigated using the Hirshfeld-I atoms-in-molecules method.[6] The evolution of the color center related bands is traced as function of the strain, and ZPL and defect formation energy was determined for neutral (GeV^0) and charged (GeV^+ & GeV^-) color centers. Combining all these results provides a clear picture of the relationship between the ZPL-position and lattice strain, which is essential for understanding the behaviour under experimental conditions in nano-crystalline diamond thin films.

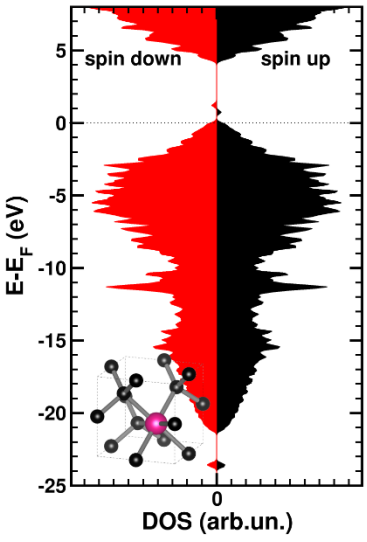

Figure 1: Density of states of the GeV^0 color center in a 5×5×5 conventional super cell.

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